Tutorial 1

Programming and Data Science

Task 1

a) We have prepared an Element class (similar to the one in the lecture script) in the file element.py. Import everything from that file. This should create instances of the Element class for most elements in the periodic table. These instances should have more attributes as what we saw before. Use the dir function to check, which attributes are available.

b) Create a plot of the atomic radius versus the electronegativity for all alkaline and earth alkaline metals (group I and II). Do you see any trends?

c) Calculate the Mulliken electronegativity for some elements of your choice and plot it versus the electronegativity values stored in the classes. Do the values align? Is the relative ordering of the elements the same?

Mulliken electronegativity

$$\chi^M = \frac{(\text{Electron affinity} - \text{Ionization Energy})}{2} \tag{1}$$

Mulliken to Pauling electronegativity conversion

$$\chi^P = 1.35 \times {\chi^M}^{0.5} - 1.37 \tag{2}$$

Task 2

a) Calculate the ionic character of some diatomic bonds. Strings corresponding to element combinations are provided in the file "experimental_data.py". Just copy over the list from there into your code.

Ionic character according to Pauling

$$IC = 1 - e^{-\frac{1}{4}(\chi_A^P - \chi_B^P)^2} \times 100 \tag{3}$$

where χ_A^P is the Pauling electronegativity of element A.

with both energies given in eV. Hint: The names of the bonds are strings. First split the into the names of the elements. Then use these element names to find the correct element instances. Here, the builtin function globals() might come in handy.

b) Can you reproduce the figure below, which shows the ionic character of a bond versus the difference in electronegativity between the two atoms. The experimental data points are also given in the file "experimental_data.py". Add them as a scatter plot.

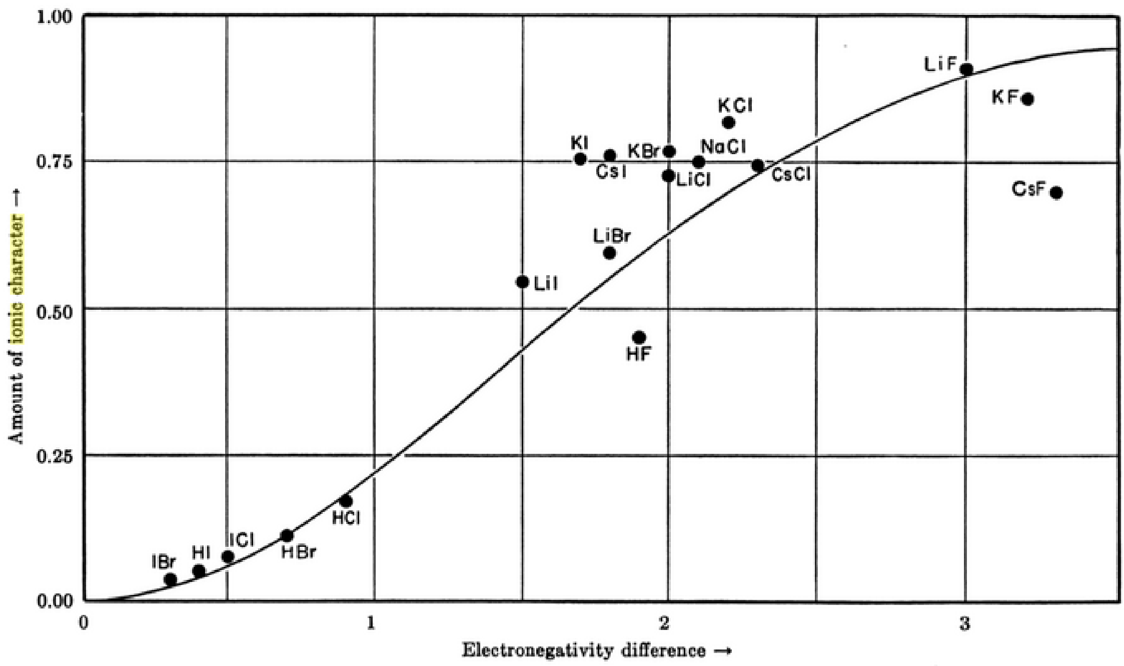

FIG. 3-8.—Curve relating the amount of ionic character of a bond to the electronegativity difference of the two atoms. Experimental points, based upon observed values of the electric dipole moment of diatomic molecules, are shown for 18 bonds.

Source: Pauling, Linus. *The nature of the chemical bond and the structure of molecules and crystals: an introduction to modern structural chemistry.* Vol. 18. Cornell university press, **1960**.